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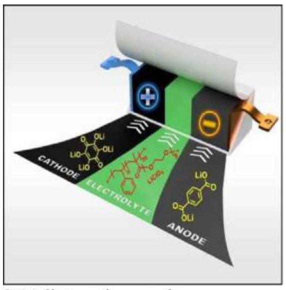
p-Conjugated Molecules: From Structure to Function

Paolo Samor%,*[a] Xinliang Feng,*[b] and Davide Bonifazi*[c]

Since the discovery and development of conductive polymers in the 1970s, which led to the award of the Nobel Prize in Chemistry 2000 to Alan. J. Heeger, Alan. G. MacDiarmid, and Hideki Shirakawa, an ever-increasing effort is being devoted to the science and technology of p-conjugated molecules and macromolecules. These systems display unique properties that make them appealing for a multitude of applications in optoelectronics, photonics, energy, and (bio)sensing. Compared to their inorganic counterparts, the greatest advantages of p-conjugated (macro)molecules lie in the molecular-level tunability of their optoelectronic properties and their processability into thin films through cheap and easily scalable methods. Further-more, macromolecular derivatives can feature mechanical properties (flexibility, toughness, malleability, elasticity, etc.) typical of plastics thus making it possible to fabricate nonpla-nar and even flexible yet robust devices.

The fabrication and technology of plastic optoelectronics is an area of intense international investigation where one of the ultimate goals is to develop smart and multifunctional devices such as LEDs, solar cells, field-effect transistors, and related applications in flexible active-matrix electronic-paper displays, sensing, and radiofrequency identification (RDIF) tags. The knowledge developed in this field will also lead to potential technological breakthroughs in organic nanophotonics, nanoelectronics, spintronics, and data-storage, as well as novel approaches to smart textiles, medical diagnostic tools (e.g. lab-on-a-chip), biocompatible devices (from artificial retinas to syn-thetic muscles), and flexible batteries.

At the basis of this interdisciplinary research endeavor, one can find the synthesis of more and more sophisticated 1D, 2D, and 3D (macro)molecular building blocks that are designed to exhibit specific physical and chemical properties. In particular, the synthesis of such systems that possess different structures and dimensionalities, as well as being characterized by multi-ple and regiospecific substitutions with functional groups at



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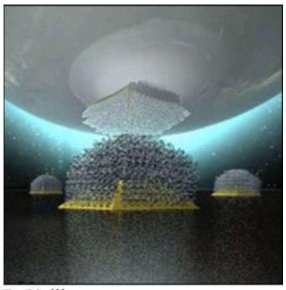

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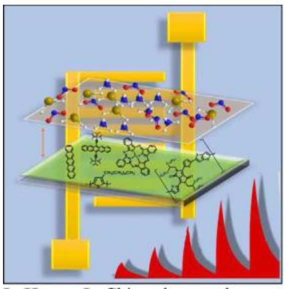
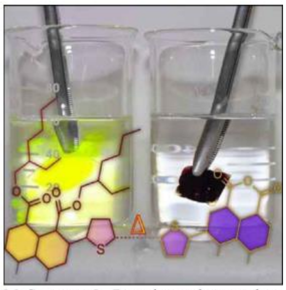


L. Huang, L. Chi, and co-workers



M. Sommer, L. Beverina and co-workers

the core, in the scaffold and/or in the periphery, makes it possible to improve fundamental photophysical properties, namely excitation energy and electron transfer. This will allow, among others, tuning of absorption and emission properties, increases in thermal and (photo)chemical stability, enhancement of molar absorptivities and fluorescence quantum efficiencies, and generation of nonlinear optical responses.

It is widely established that the properties of organic and polymeric materials, either arranged as thin or thicker films, strongly depend on the organization at the supramolecular level. This means that the materials and device properties are determined not only by those intrinsic to the structure of the constituent molecules (molecular level) but also by those resulting from the interactions between adjacent molecules (supramolecular level). In particular, there are many physical properties, such as charge transfer (through hopping), charge split and recombination, and exciton diffusion, to name but a few, that depend more critically on the supramolecular organization. In light of this, the self-assembly and self-organization of macromolecules at surfaces and interfaces are key, also to enabling optimal interfacial properties such as charge injection and extraction via energy matching. Such a control over these physical properties at the molecular and supramolecular level is therefore of paramount importance for improved device performance.

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This Special Issue highlights some of the most enlightening approaches on the synthesis of novel conjugated (macro)molecules with special properties arising from their p-conjugation, their processing and self-assembly at surfaces and interfaces, their multiscale analysis of the relevant physical and chemical properties, and their integration in optoelectronic, photovoltaics, batteries, and chemical sensing devices. Images from the Review and Minireview articles, as well as the paper featured on the cover are shown here.

We believe that this Special Issue will offer readers some inspiring examples of the wide scope of this field of science and technology and hopefully convey the enthusiasm of the scientists involved in this research. We are most grateful to all contributing authors for their effort in highlighting and addressing the key questions in this highly dynamic field of chemistry at its interface with physics and engineering, in the interdisciplinary realms of materials and nanoscience.

Xinliang Feng is Full Professor and Head of the Chair of Molecular Functional Materials at the Technische Universit t Dresden. His current scientific interests include organic synthetic methodology, organic synthesis and supramolecular chemistry of p-conjugated systems, bottom-up synthesis and top-down fabrication of graphene and graphene nanoribbons, 2D polymers and supramolecular polymers, 2D carbon-rich conjugated polymers for optoelectronic applications, energy storage and conversion, and new energy devices and technologies. He has been awarded several prestigious prizes such as IUPAC Prize for Young Chemists (2009), European Research Council (ERC) Starting Grant Award (2012), Journal of Materials Chemistry Lectureship Award (2013), ChemComm Emerging Investigator Lectureship (2014), Highly Cited Researcher (Thomson Reuters, 2014–2018), Small Young Innovator Award (2017), Hamburg Science Award (2017), EU-40 Materials Prize (2018), and an ERC Consolidator Grant Award (2018). He is a Fellow of the Royal Society of Chemistry (FRSC), Member of the European Academy of Sciences and Member of the Academia Europaea. He is the Head of ESF Young Research Group “Graphene Center Dresden”, and Working Package Leader of WP Functional Foams & Coatings for European Commission’s pilot project “Graphene Flagship”.

Paolo Samor$ is Distinguished Professor at the Universit de Strasbourg and Director of the Institut de Science et d’Ing nierie Supramol culaires (ISIS). He is Fellow of the Royal Society of Chemistry (FRSC), Foreign Member of the Royal Flemish Academy of Belgium for Science and the Arts (KVAB), Fellow of the European Academy of Sciences (EURASC), Member of the Academia Europaea and Junior Member of the Institut Universitaire de France (IUF). His research interests encompass supramolecular sciences, nanochemistry and materials chemistry with a specific focus on p-conjugated macromolecules, graphene and other 2D materials as well as functional hybrid nanomaterials for application in opto-electronics, energy and sensing. His work has been recognized with various prizes, including the Young Scientist Award by E-MRS (1998) and MRS (2000), the IUPAC Prize for Young Chemists (2001), the ERC Starting Grant (2010), the CNRS Silver Medal (2012), the Spanish–French CatalQn–Sabatier Prize (2017), the German–French Georg Wittig–Victor Grignard Prize (2017), the Surface and Interfaces Award by the RSC (2018) and the Blaise Pascal Medal in Materials Science by EURASC (2018), the Pierre S4e Prize of the French Chemical Society (2018), and an ERC Advanced Grant (2019).

Davide Bonifazi is Chair Professor of Organic Supramolecular Chemistry in the School of Chemistry at Cardiff University (UK). His current research interests are focused on the creation of functional p-conjugated organic architectures in interdisciplinary projects through targeted organic synthesis, self-assembly, and self-organization of organic architectures in solution and on surfaces, physical-organic studies, material- and biobased design for optoelectronic applications, light-harvesting applications and biology. He is a Fellow of the Learned Society of Wales (2019). His work has been awarded with the Young Investigator Lectureship at the ISCHIA School of Organic Chemistry (2012), an ERC Starting Grant (2011), the G. Ciamician Medal (2010), and the ETH Silver Medallion (2005).